

## SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: BEN JACKSON Examiner #: 73489 Date: 3/3/03  
 Art Unit: 1620 Phone Number 305-6889 Serial Number: 10/069, 579  
 Mail Box and Bldg/Room Location: CM1 3619 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need. mej

\*\*\*\*\*

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Method for producing Cyanoacetic acid Esters  
 Inventors (please provide full names): Paul Hanselmann et al

Earliest Priority Filing Date: 8/30/99

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

A process for preparing cyanoacetic acid ester of formula RC(=O)CH2CO2R' comprising oxidizing alkoxypropionic acid of formula ROCH2CH2CO2R'' wherein R is optionally subst. linear alkyl or branched C<sub>1</sub>-8 alkyl or an aryl of C<sub>1</sub>-4 alkyl group, R' is oxygen or oxygen bearing group and R'' is in the presence of a catalyst based on lead or one of the transition metals.

Jan Delavai  
 Reference Librarian  
 Biotechnology & Chemical Library  
 CM1 1E07 - 703-308-4498  
 jan.delavai@uspto.gov

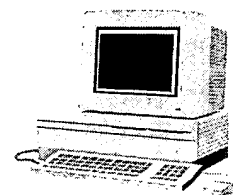
## STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>an</u>	NA Sequence (#) _____	STN <u>✓</u>
Searcher Phone #: <u>4478</u>	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) <u>L</u>	Questel/Orbit _____
Date Searcher Picked Up: <u>3/10/03</u>	Bibliographic _____	Dr.Link _____
Date Completed: <u>3/10/03</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: _____	Fulltext _____	Sequence Systems _____
Clerical Prep Time: <u>10</u>	Patent Family _____	WWW/Internet _____
Online Time: <u>125</u>	Other _____	Other (specify) _____

# BioTech-Chem Library

## Search Results

### Feedback Form (Optional)



Scientific & Technical Information Center

The search results generated for your recent request are attached. If you have any questions or comments (compliments or complaints) about the scope or the results of the search, please contact *the BioTech-Chem searcher* who conducted the search *or contact*:

**Mary Hale, Supervisor, 308-4258**  
CM-1 Room 1E01

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#### *Voluntary Results Feedback Form*

➤ *I am an examiner in Workgroup:* (Example: 1610)

➤ *Relevant prior art **found**, search results used as follows:*

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

*Types of relevant prior art found:*

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature  
(journal articles, conference proceedings, new product announcements etc.)

➤ *Relevant prior art **not found**:*

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Search results were not useful in determining patentability or understanding the invention.

**Other Comments:**

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Drop off completed forms at the **Circulation Desk CM-1**, or send to Mary Hale, **CM1-1E01** or e-mail **mary.hale@uspto.gov**.

=> fil casreact  
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FILE CONTENT:1907 - 9 Mar 2003 VOL 138 ISS 10

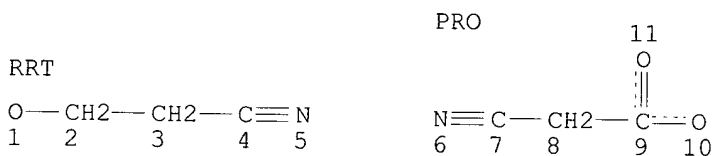
Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> d sta que l5  
 L3 STR



NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE  
 L5 2 SEA FILE=CASREACT SSS FUL L3 ( 4 REACTIONS)

100.0% DONE 10260 VERIFIED 4 HIT RXNS 2 DOCS  
 SEARCH TIME: 00.00.01

=> d l5 bib abs fhlt retable tot

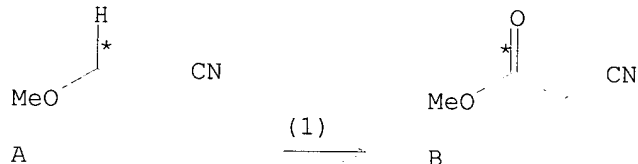
L5 ANSWER 1 OF 2 CASREACT COPYRIGHT 2003 ACS  
 AN 134:207549 CASREACT  
 TI Oxidative method and catalysts for producing cyanoacetate esters from  
 3-(alkoxy)propionitriles  
 IN Hanselmann, Paul; Hildbrand, Stefan  
 PA Lonza A.-G., Switz.  
 SO PCT Int. Appl., 14 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA German

Jan 2004  
 Reference Librarian  
 Biotechnology & Chemical Library  
 500 1507-7014  
 1000 1000 1000

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001016092	A1	20010308	WO 2000-EP8397	20000829
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1208081	A1	20020529	EP 2000-964050	20000829
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
PRAI	EP 1999-117033		19990830		
	US 2000-185372P		20000228		
	WO 2000-EP8397		20000829		
OS	MARPAT 134:207549				
AB	Cyanoacetate esters NCCH <sub>2</sub> CO <sub>2</sub> R [R = (un)substituted (un)branched C1-8 alkyl, arylalkyl] (e.g., Me 2-cyanoacetate) are prepd. in high yield and selectivity by the oxidn. of 3-(alkoxy)propionitriles RO(CH <sub>2</sub> ) <sub>2</sub> CN (e.g., 3-methoxypropionitrile) in the presence of a catalyst based on lead or on one of the transition metals (e.g., cobalt diacetate tetrahydrate) using oxygen or an oxygen-forming reagent (e.g., N-hydroxyphthalimide).				

RX(1) OF 3      A ==&gt; B



RX(1)      RCT    A 110-67-8

STAGE(1)

RGT    C 524-38-9 N-Hydroxyphthalimide

CAT    6147-53-1 Acetic acid, cobalt(2+) salt, tetrahydrate

SOL    64-19-7 AcOH

STAGE(2)

RGT    D 7782-44-7 O<sub>2</sub>

PRO    B 105-34-0

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Catalytcca Inc	1992			WO 9212962 A	CAPLUS
Matsui, K	1984			US 4438041 A	CAPLUS
Wermeckes, B	1985	118	3771	CHEM BER	CAPLUS
Wermeckes, B	1985	30	1491	ELECTROCHIM ACTA	CAPLUS

L5      ANSWER 2 OF 2    CASREACT    COPYRIGHT 2003 ACS

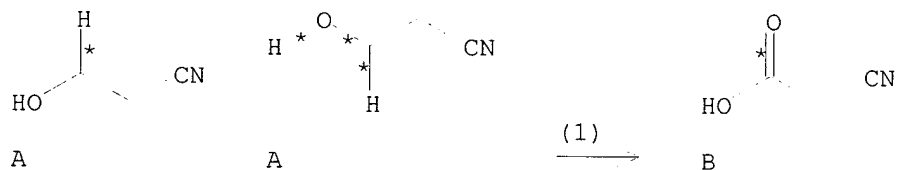
AN      103:214838    CASREACT

TI      Anodic oxidation of 2-cyanoethanol to cyanoacetic acid

AU      Wermeckes, Bernd; Beck, Fritz

CS GH, Univ. Duisburg, Duisburg, D-4100/1, Fed. Rep. Ger.  
 SO Chemische Berichte (1985), 118(9), 3771-80  
 CODEN: CHBEAM; ISSN: 0009-2940  
 DT Journal  
 LA German  
 AB 2-Cyanoethanol was oxidized electrochem. to cyanoacetic acid in aq. H<sub>2</sub>SO<sub>4</sub> at Pt and PbO<sub>2</sub> anodes (current densities of 30-200 mA cm<sup>-2</sup>). Current efficiencies and material yields were up to 60%. Side products were HCN (via an anodic attack at .beta.-CH<sub>2</sub>) and cyanoacetaldehyde, with 8-15 and 3-13% current efficiencies on Pt. In principle, HCN can be recycled to new starting material and cyanoacetaldehyde to yield further product. Electrooxidn. at Pt takes place at an anode which is partially covered with platinum oxides. High over-voltages are interpreted in terms of a voltage drop in a rigid org. adsorbate layer.

RX(1) OF 1 2 A ==> B + C



C

RX(1) RCT A 109-78-4  
 RGT D 7664-93-9 H<sub>2</sub>SO<sub>4</sub>  
 PRO B 372-09-8, C 6162-76-1  
 SOL 7732-18-5 Water  
 NTE Anodic oxidn.

=> fil reg

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STRUCTURE FILE UPDATES: 9 MAR 2003 HIGHEST RN 497220-90-3  
 DICTIONARY FILE UPDATES: 9 MAR 2003 HIGHEST RN 497220-90-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

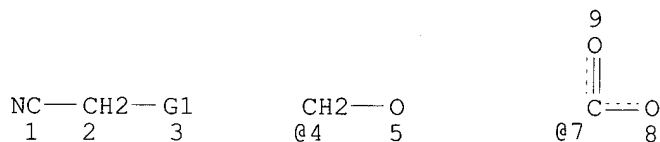
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties

in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

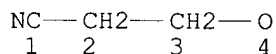
=> d sta que l11  
 L6 STR



VAR G1=4/7  
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 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
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 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE  
 L8 14129 SEA FILE=REGISTRY SSS FUL L6  
 L9 STR



NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

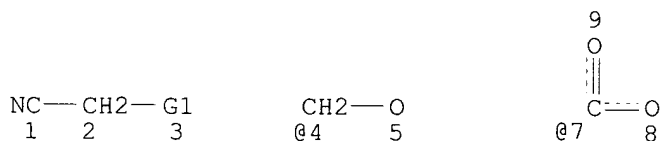
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 NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE  
 L11 13071 SEA FILE=REGISTRY SUB=L8 SSS FUL L9

100.0% PROCESSED 13996 ITERATIONS  
 SEARCH TIME: 00.00.01

13071 ANSWERS

=> d sta que l13  
 L6 STR

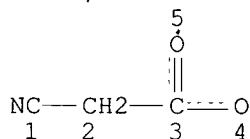


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 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
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 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L8 14129 SEA FILE=REGISTRY SSS FUL L6  
L12 STR



NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE  
L13 1059 SEA FILE=REGISTRY SUB=L8 SSS FUL L12

100.0% PROCESSED 4883 ITERATIONS  
SEARCH TIME: 00.00.01

1059 ANSWERS

=> d his

(FILE 'HOME' ENTERED AT 07:40:07 ON 10 MAR 2003)  
SET COST OFF

FILE 'CASREACT' ENTERED AT 07:40:32 ON 10 MAR 2003

L1 STR  
L2 0 S L1  
L3 STR L1  
L4 0 S L3  
L5 2 S L3 FUL  
SAV L5 SACKY069/A

FILE 'CASREACT' ENTERED AT 07:43:47 ON 10 MAR 2003

FILE 'REGISTRY' ENTERED AT 07:44:12 ON 10 MAR 2003

L6 STR  
L7 50 S L6  
L8 14129 S L6 FUL  
SAV TEMP L8 SACKY069A/A  
L9 STR  
L10 50 S L9 SAM SUB=L8  
L11 13071 S L9 FUL SUB=L8  
SAV TEMP L11 SACKY069B/A  
L12 STR L9  
L13 1059 S L12 FUL SUB=L8  
SAV L13 SACKY069C/A  
E COBALT/CN  
L14 1 S E3  
L15 9 S COBALT (L) ACETATE (L) TETRAHYDRATE  
L16 1 S L15 AND C2H4O2 AND H2O AND 3/NC  
L17 17 S 64-19-7/CRN AND CO/ELS AND H2O  
L18 14 S L17 AND 3/NC  
L19 10 S L18 NOT N/ELS  
E LEAD/CN  
L20 1 S E3  
E T/HP  
E TR/HP

E T/PG  
E A/PG  
L21 6423 S E23-E25 AND 1/ELC.SUB  
L22 3889 S L21 NOT ISOTOPE  
L23 1340 S L22 AND 1/ATC  
L24 38 S L23 NOT ION

FILE 'HCAPLUS' ENTERED AT 07:52:34 ON 10 MAR 2003

L25 7333 S L13  
L26 8502 S L11  
L27 79 S L25 AND L26  
L28 2 S L27 AND L14,L16,L19,L20,L24  
L29 13 S L13/P AND L27  
L30 4517 S L26 (L) (RCT OR RACT OR RGT)/RL  
L31 41 S L30 AND L27  
L32 5 S L29 AND L31  
L33 5 S L28,L32

FILE 'REGISTRY' ENTERED AT 07:55:12 ON 10 MAR 2003

L34 1 S OXYGEN/CN

FILE 'HCAPLUS' ENTERED AT 07:55:17 ON 10 MAR 2003

L35 1 S L27 AND L34  
L36 5 S L33,L35  
E HANSELMANN P/AU  
L37 17 S E4  
E HILDBRAND S/AU  
L38 14 S E4  
E LONZA/PA,CS  
L39 1853 S E3,E4  
L40 1 S L37,L38,L39 AND L27  
L41 6 S L37,L38,L39 AND L26  
L42 5 S L36,L40  
L43 5 S L41 NOT L42

FILE 'USPATFULL, USPAT2' ENTERED AT 07:56:53 ON 10 MAR 2003

L44 1971 S L11  
L45 1636 S L13  
L46 25 S L44 AND L45  
L47 0 S L46 AND L14,L16,L19,L20,L24,L34  
L48 21 S L46 AND (PB OR LEAD OR CO OR COBALT OR TRANSITION METAL OR OX  
L49 6 S L11/P AND L46  
L50 6 S L48 AND L49  
L51 0 S L49 AND COBALT

FILE 'IFIPAT' ENTERED AT 08:00:48 ON 10 MAR 2003

FILE 'REGISTRY' ENTERED AT 08:01:32 ON 10 MAR 2003

=> fil hcaplus

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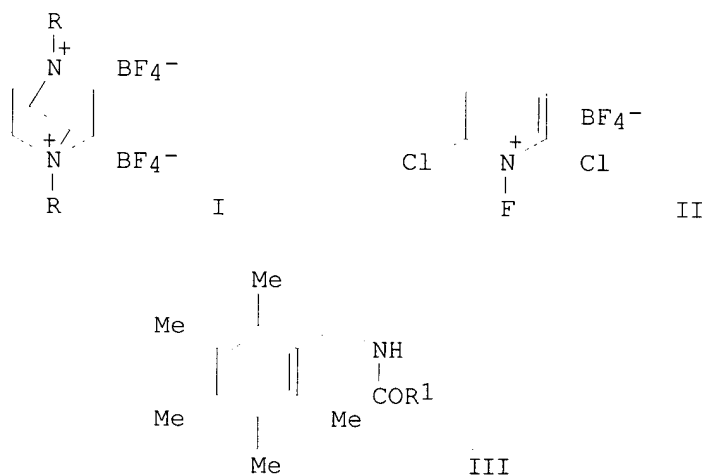
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FILE COVERS 1907 - 10 Mar 2003 VOL 138 ISS 11  
FILE LAST UPDATED: 9 Mar 2003 (20030309/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

L42 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2003 ACS  
AN 2001:508660 HCAPLUS  
DN 135:272730  
TI Effective and versatile functionalisation of hexamethylbenzene using N-F  
reagents  
AU Stavber, Stojan; Kralj, Petra; Zupan, Marko  
CS Laboratory for Organic and Bioorganic Chemistry, "Jozef Stefan" Institute  
and Department of Chemistry, University of Ljubljana, Ljubljana, 1000,  
Slovenia  
SO Synlett (2001), (7), 1152-1154  
CODEN: SYNLES; ISSN: 0936-5214  
PB Georg Thieme Verlag  
DT Journal  
LA English  
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
OS CASREACT 135:272730  
GI



AB Effective direct introduction of alkoxy, amino, azido or halogeno functional groups on the benzylic position in hexamethylbenzene was mediated by the electrophilic fluorinating (N-F) reagents I (R = ClCH<sub>2</sub>, HO), (PhSO<sub>2</sub>)<sub>2</sub>NF and II in the presence of alcs., carboxylic acids, cyanides or trimethylsilyl derivs. as sources of an external nucleophile. Thus, aryl amides III [R<sub>1</sub> = Et, Me(CH<sub>2</sub>)<sub>4</sub>, MeCH, cyclopropyl, MeOCH<sub>2</sub>, MeO<sub>2</sub>CCH<sub>2</sub>, EtO<sub>2</sub>CCH<sub>2</sub>, Ph, 4-MeO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>, PhCH<sub>2</sub>] were prepd. from the reaction of hexamethylbenzene and R<sub>1</sub>CONH<sub>2</sub> mediated by I (R = ClCH<sub>2</sub>) in 65-98% yield.

ST ether benzyl prepn; nucleophile methylbenzene substitution electrophilic

fluorinating reagent mediated; etherification alc methylbenzene  
electrophilic fluorinating reagent mediated; amidation nitrile  
methylbenzene electrophilic fluorinating reagent mediated; amide benzyl  
prepn; benzylic functionalisation methylbenzene electrophilic fluorinating  
reagent

- IT Fluorination  
(agents, electrophilic; prepn. of pentamethylphenylmethyl ethers and  
amides via electrophilic fluorinating reagent-mediated etherification  
and amidation reaction of hexamethylbenzene with alcs. and nitriles)
- IT Amides, preparation  
Ethers, preparation  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(benzyl; prepn. of pentamethylphenylmethyl ethers and amides via  
electrophilic fluorinating reagent-mediated etherification and  
amidation reaction of hexamethylbenzene with alcs. and nitriles)
- IT Amidation  
(prepn. of pentamethylphenylmethyl amides via electrophilic  
fluorinating reagent-mediated amidation of hexamethylbenzene with  
nitriles)
- IT Nucleophiles  
(prepn. of pentamethylphenylmethyl derivs. via electrophilic  
fluorinating reagent-mediated substitution of hexamethylbenzene with  
nucleophiles)
- IT Alcohols, reactions  
Nitriles, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of pentamethylphenylmethyl ethers and amides via electrophilic  
fluorinating reagent-mediated etherification and amidation reaction of  
hexamethylbenzene with alcs. and nitriles)
- IT Substitution reaction  
(prepn. of pentamethylphenylmethyl ethers and amides via electrophilic  
fluorinating reagent-mediated substitution reaction of  
hexamethylbenzene with alcs. and nitriles)
- IT Etherification  
(prepn. of pentamethylphenylmethyl ethers via electrophilic  
fluorinating reagent-mediated etherification of hexamethylbenzene with  
alcs.)
- IT 109-78-4, 2-Cyanoethanol  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of pentamethylphenylmethyl amide and ether via electrophilic  
fluorinating reagent-mediated substitution reaction of  
hexamethylbenzene with cyanoethanol in TFA and MeCN)
- IT 363148-38-3P 363148-39-4P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of pentamethylphenylmethyl amide and ether via electrophilic  
fluorinating reagent-mediated substitution reaction of  
hexamethylbenzene with cyanoethanol in TFA and MeCN)
- IT 7062-95-5, Potassium cyanoacetate  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating  
reagent-mediated substitution reaction of hexamethylbenzene with K  
cyanoacetate in MeCN)
- IT 363148-37-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating  
reagent-mediated substitution reaction of hexamethylbenzene with K  
cyanoacetate in MeCN)
- IT 372-09-8, 2-Cyanoacetic acid  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating  
reagent-mediated substitution reaction of hexamethylbenzene with  
cyanoacetic acid in TFA)
- IT 363148-36-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with cyanoacetic acid in TFA)

IT 484-65-1P 243118-23-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of pentamethylphenylmethyl azide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with TMS azide)

IT 19936-85-7P 35843-80-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of pentamethylphenylmethyl esters via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with carboxylic acids)

IT 67-63-0, 2-Propanol, reactions 75-89-8, 2,2,2-Trifluoroethanol 78-82-0, 2-Cyanopropane 87-85-4, Hexamethylbenzene 96-41-3, Cyclopentanol 100-47-0, Benzonitrile, reactions 100-51-6, Benzyl alcohol, reactions 105-34-0, Methyl 2-cyanoacetate 105-56-6, Ethyl 2-cyanoacetate 107-12-0, Propionitrile 109-86-4, 2-Methoxyethanol 111-27-3, 1-Hexanol, reactions 140-29-4, Benzonitrile 628-73-9, Hexanenitrile 1129-35-7, Methyl 4-cyanobenzoate 1738-36-9, Methoxyacetone nitrile 5500-21-0, Cyclopropanenitrile 133745-75-2, N-Fluorobenzenesulfonimide 140623-89-8, N-Fluoro-2,6-dichloropyridinium tetrafluoroborate 140681-55-6, Selectfluor 172090-26-5, 1-Fluoro-4-hydroxy-1,4-diazoniabicyclo[2.2.2]octane bis(tetrafluoroborate)

RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of pentamethylphenylmethyl ethers and amides via electrophilic fluorinating reagent-mediated etherification and amidation reaction of hexamethylbenzene with alcs. and nitriles)

IT 64512-95-4P 363148-21-4P 363148-22-5P 363148-23-6P 363148-24-7P  
363148-25-8P 363148-26-9P 363148-27-0P 363148-28-1P 363148-29-2P  
363148-30-5P 363148-31-6P 363148-32-7P 363148-33-8P 363148-34-9P  
363148-35-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of pentamethylphenylmethyl ethers and amides via electrophilic fluorinating reagent-mediated etherification and amidation reaction of hexamethylbenzene with alcs. and nitriles)

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE

- (1) Anon; Methods of Organic Chemistry (Houben-Weyl) 1999, VE 10a and 10b
- (2) Bewick, A; Liebigs Ann Chem 1978, P41 HCAPLUS
- (3) Bishop, R; Comprehensive Organic Synthesis 1991, V6 HCAPLUS
- (4) Dalla Cort, A; J Chem Res S 1983, P44 HCAPLUS
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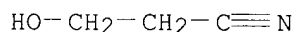
IT 109-78-4, 2-Cyanoethanol

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of pentamethylphenylmethyl amide and ether via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with cyanoethanol in TFA and MeCN)

RN 109-78-4 HCAPLUS

CN Propanenitrile, 3-hydroxy- (9CI) (CA INDEX NAME)



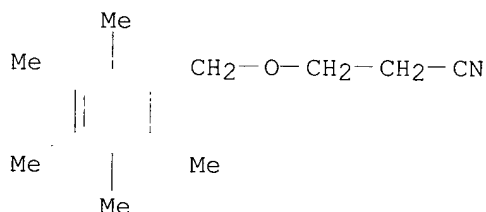
IT 363148-38-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of pentamethylphenylmethyl amide and ether via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with cyanoethanol in TFA and MeCN)

RN 363148-38-3 HCAPLUS

CN Propanenitrile, 3-[(pentamethylphenyl)methoxy]- (9CI) (CA INDEX NAME)



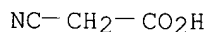
IT 7062-95-5, Potassium cyanoacetate

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with K cyanoacetate in MeCN)

RN 7062-95-5 HCAPLUS

CN Acetic acid, cyano-, potassium salt (8CI, 9CI) (CA INDEX NAME)



● K

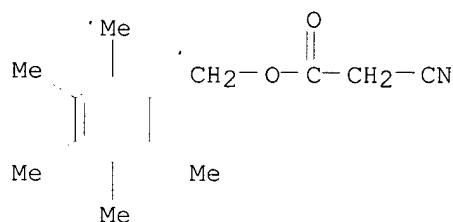
IT 363148-37-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

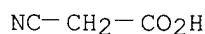
(prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating reagent-mediated substitution reaction of hexamethylbenzene with K cyanoacetate in MeCN)

RN 363148-37-2 HCAPLUS

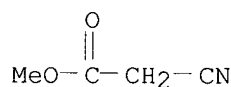
CN Acetic acid, cyano-, (pentamethylphenyl)methyl ester (9CI) (CA INDEX NAME)



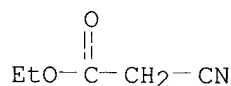
IT **372-09-8**, 2-Cyanoacetic acid  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of pentamethylphenylmethyl amide via electrophilic fluorinating  
 reagent-mediated substitution reaction of hexamethylbenzene with  
 cyanoacetic acid in TFA)  
 RN 372-09-8 HCAPLUS  
 CN Acetic acid, cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



IT **105-34-0**, Methyl 2-cyanoacetate **105-56-6**, Ethyl  
 2-cyanoacetate  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of pentamethylphenylmethyl ethers and amides via electrophilic  
 fluorinating reagent-mediated etherification and amidation reaction of  
 hexamethylbenzene with alcs. and nitriles)  
 RN 105-34-0 HCAPLUS  
 CN Acetic acid, cyano-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 105-56-6 HCAPLUS  
 CN Acetic acid, cyano-, ethyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)



L42 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2003 ACS  
 AN 2001:167957 HCAPLUS  
 DN 134:207549  
 TI Oxidative method and catalysts for producing cyanoacetate esters from  
 3-(alkoxy)propionitriles  
 IN **Hanselmann, Paul; Hildbrand, Stefan**  
 PA **Lonza A.-G.**, Switz.  
 SO PCT Int. Appl., 14 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA German  
 IC ICM C07C253-30  
 ICS C07C255-19  
 CC 23-17 (Aliphatic Compounds)  
 Section cross-reference(s): 45, 67

FAN.CNT 1

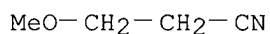
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001016092	A1	20010308	WO 2000-EP8397	20000829
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1208081	A1	20020529	EP 2000-964050	20000829
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
PRAI	EP 1999-117033	A	19990830		
	US 2000-185372P	P	20000228		
	WO 2000-EP8397	W	20000829		
OS	CASREACT 134:207549; MARPAT 134:207549				
AB	Cyanoacetate esters NCCH <sub>2</sub> CO <sub>2</sub> R [R = (un)substituted (un)branched C1-8 alkyl, arylalkyl] (e.g., Me 2-cyanoacetate) are prepd. in high yield and selectivity by the oxidn. of 3-(alkoxy)propionitriles RO(CH <sub>2</sub> ) <sub>2</sub> CN (e.g., 3-methoxypropionitrile) in the presence of a catalyst based on lead or on one of the transition metals (e.g., cobalt diacetate tetrahydrate) using oxygen or an oxygen-forming reagent (e.g., N-hydroxyphthalimide).				
ST	cyanoacetate ester prepn oxidn alkoxypropionitrile; catalyst oxidn alkoxypropionitrile prepn cyanoacetate ester; methyl cyanoacetate prepn methoxypropionitrile oxidn				
IT	Organic compounds, reactions				
	RL: RCT (Reactant); RACT (Reactant or reagent) (cyano, 3-(alkoxy)propionitriles; oxidative method and catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)				
IT	Oxidation				
	(liq.-phase, .0; of 3-(alkoxy)propionitriles into cyanoacetate esters)				
IT	Oxidation catalysts				
	(liq.-phase; lead or transition metals for the conversion of 3-(alkoxy)propionitriles into cyanoacetate esters)				
IT	Transition metals, uses				
	RL: CAT (Catalyst use); USES (Uses) (oxidn. catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)				
IT	110-67-8, 3-Methoxypropionitrile 524-38-9, N-Hydroxyphthalimide 2141-62-0, 3-Ethoxypropionitrile 7782-44-7, Oxygen, reactions				
	RL: RCT (Reactant); RACT (Reactant or reagent) (oxidative method and catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)				
IT	105-34-0P, Methyl 2-cyanoacetate 105-56-6P, Ethyl 2-cyanoacetate				
	RL: SPN (Synthetic preparation); PREP (Preparation) (oxidative method and catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)				
IT	6147-53-1, Cobalt diacetate tetrahydrate 7439-92-1, Lead, uses				
	RL: CAT (Catalyst use); USES (Uses) (oxidn. catalysts for producing cyanoacetate esters from 3-(alkoxy)propionitriles)				

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

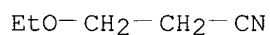
RE

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IT 110-67-8, 3-Methoxypropionitrile 2141-62-0,  
3-Ethoxypropionitrile 7782-44-7, Oxygen, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidative method and catalysts for producing cyanoacetate esters from  
3-(alkoxy)propionitriles)  
RN 110-67-8 HCAPLUS  
CN Propanenitrile, 3-methoxy- (9CI) (CA INDEX NAME)



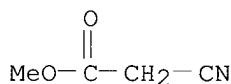
RN 2141-62-0 HCAPLUS  
CN Propanenitrile, 3-ethoxy- (9CI) (CA INDEX NAME)



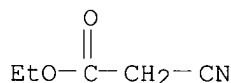
RN 7782-44-7 HCAPLUS  
CN Oxygen (8CI, 9CI) (CA INDEX NAME)



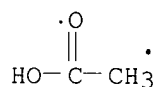
IT 105-34-0P, Methyl 2-cyanoacetate 105-56-6P, Ethyl  
2-cyanoacetate  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(oxidative method and catalysts for producing cyanoacetate esters from  
3-(alkoxy)propionitriles)  
RN 105-34-0 HCAPLUS  
CN Acetic acid, cyano-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 105-56-6 HCAPLUS  
CN Acetic acid, cyano-, ethyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 6147-53-1, Cobalt diacetate tetrahydrate 7439-92-1,  
Lead, uses  
RL: CAT (Catalyst use); USES (Uses)  
(oxidn. catalysts for producing cyanoacetate esters from  
3-(alkoxy)propionitriles)  
RN 6147-53-1 HCAPLUS  
CN Acetic acid, cobalt(2+) salt, tetrahydrate (8CI, 9CI) (CA INDEX NAME)



● 1/2 Co(II)

● 2 H<sub>2</sub>O

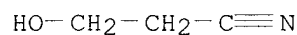
RN 7439-92-1 HCAPLUS  
CN Lead (8CI, 9CI) (CA INDEX NAME)

Pb

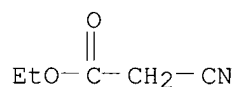
L42 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2003 ACS  
AN 1988:94057 HCAPLUS  
DN 108:94057  
TI Convenient synthesis for selectively isotopically labeled acrylonitriles  
AU Van den Berg, E. M. M.; Richardson, E. E.; Lugtenburg, J.; Jenneskens, L. W.  
CS Gorlaeus Lab., Univ. Leiden, Leiden, 2300 RA, Neth.  
SO Synthetic Communications (1987), 17(10), 1189-98  
CODEN: SYNCAV; ISSN: 0039-7911  
DT Journal  
LA English  
CC 23-19 (Aliphatic Compounds)  
OS CASREACT 108:94057  
AB Short syntheses of CH<sub>2</sub>:CHCN (I) and HOCH<sub>2</sub>CH<sub>2</sub>CN (II) which can be used to prep. isotopically labeled I are reported. Thus, HOCH<sub>2</sub>CH<sub>2</sub>Br reacted with KCN to give II, which was treated with Ac<sub>2</sub>O to give AcOCH<sub>2</sub>CH<sub>2</sub>CN. Flash vacuum thermolysis of the latter compd. gave I in near quant. yield.  
ST labeled acrylonitrile prepn; cyanoethyl acetate prepn elimination  
IT Elimination reaction  
    . (of cyanoethyl acetate, acrylonitrile from)  
IT 105-58-8, Diethyl carbonate  
    RL: RCT (Reactant); RACT (Reactant or reagent)  
        (acylation by, of lithiated acetonitrile)  
IT 75-05-8, Acetonitrile, reactions  
    RL: RCT (Reactant); RACT (Reactant or reagent)  
        (lithiation and acylation of, with di-Et carbonate)  
IT 109-78-4P, 2-Cyanoethanol  
    RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**  
        (prepn. and acetylation of)  
IT 105-56-6P, Ethyl .alpha.-cyanoacetate  
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
        (prepn. and borohydride redn. of)  
IT 5325-93-9P, 2-Cyanoethyl acetate  
    RL: SPN (Synthetic preparation); PREP (Preparation)  
        (prepn. and elimination of acetic acid from)  
IT 372-09-8P  
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)



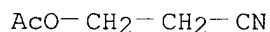
(prepn. and esterification of)  
 IT 107-13-1P, Acrylonitrile, preparation  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of, as model synthesis of labeled derivs. of)  
 IT 79-08-3, .alpha.-Bromoacetic acid 540-51-2, 2-Bromoethanol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (substitution reaction of, with cyanide)  
 IT 109-78-4P, 2-Cyanoethanol  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation); RACT (Reactant or reagent)  
 (prepn. and acetylation of)  
 RN 109-78-4 HCAPLUS  
 CN Propanenitrile, 3-hydroxy- (9CI) (CA INDEX NAME)



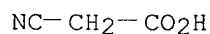
IT 105-56-6P, Ethyl .alpha.-cyanoacetate  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and borohydride redn. of)  
 RN 105-56-6 HCAPLUS  
 CN Acetic acid, cyano-, ethyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 5325-93-9P, 2-Cyanoethyl acetate  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. and elimination of acetic acid from)  
 RN 5325-93-9 HCAPLUS  
 CN Propanenitrile, 3-(acetyloxy)- (9CI) (CA INDEX NAME)



IT 372-09-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and esterification of)  
 RN 372-09-8 HCAPLUS  
 CN Acetic acid, cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)



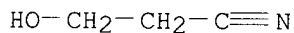
L42 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2003 ACS  
 AN 1986:41890 HCAPLUS  
 DN 104:41890  
 TI Anodic oxidation of .beta.-cyanoethyl ethers  
 AU Wermeckes, B.; Beck, F.  
 CS Univ. Duisburg, Duisburg, D 4100/1, Fed. Rep. Ger.  
 SO Electrochimica Acta (1985), 30(11), 1491-500  
 CODEN: ELCAAV; ISSN: 0013-4686  
 DT Journal  
 LA English

- CC 72-4 (Electrochemistry)  
Section cross-reference(s): 23
- AB Anodic oxidn. of .beta.-cyanoethyl ethers ROCH<sub>2</sub>CH<sub>2</sub>CN (R = Me, Et, tert-Bu, CH<sub>2</sub>CH<sub>2</sub>CN) was carried out in 1.6M H<sub>2</sub>SO<sub>4</sub>, using Pt and PbO<sub>2</sub> as anodes. The main products were cyanoacetic acid (CEA) and the acid corresponding to R (HCOOH for R = Me, HOAc for R = Et). In the case of R = Et (EPN), HOAc was found with current efficiencies up to 81% (at low conversions), while CEA was generated with relatively low current efficiencies .ltoreq.34%. Kinetic curves for EPN exhibit an early appearance of .beta.-oxypropionitrile (OPN), the intermediate to CEA, and acetaldehyde. Thus, the -CH<sub>2</sub> group of Et is primarily attacked to yield the semiacetal in a 2 electron oxidn., which is rapidly cleaved in acid solns. to yield the above-mentioned intermediates. HCN found as a side product is derived from anodic attack at the -CH<sub>2</sub> group adjacent to the cyano group, leading to the readily sapond. cyanohydrin. The ether reacts in the adsorbed state. This leads to large pos. potential shifts and unusual Tafel slopes of 240-300 mV decade<sup>-1</sup> due to only partial efficiency of Galvani voltage. Moreover, a partial coverage of Pt electrode with PtOx was detected even in the presence of the ether. Coincidence of PtOx-potential and initial oxidn. potential of ether leads to the proposal of a mechanism in terms of redox catalysis. Et<sub>2</sub>O is oxidized to HOAc in high yields. Thus, these findings are not restricted to .beta.-cyanoethyl ethers.
- ST cyanoethyl ether electrooxidn; methyl cyanoethyl ether electrooxidn; ethyl cyanoethyl ether electrooxidn; butyl cyanoethyl ether electrooxidn; alkyl cyanoethyl ether electrooxidn; lead oxide anode cyanoethyl ether; platinum anode cyanoethyl ether oxidn; cyanoacetic acid electroprepn cyanoethyl ether; formic acid electroprepn cyanoethyl ether; acetic acid electroprepn cyanoethyl ether
- IT Ethers, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyanoethyl, oxidn. of, electrochem., on lead oxide or platinum in sulfuric acid)
- IT Electric current  
(efficiency of, in oxidn. of .beta.-cyanoethyl ethers on lead oxide or platinum in sulfuric acid)
- IT Oxidation, electrochemical  
(of .beta.-cyanoethyl ethers, on lead oxide or platinum in sulfuric acid)
- IT Electric potential  
(oxidn., of cyano compds. in sulfuric acid)
- IT **7440-06-4**, uses and miscellaneous  
RL: USES (Uses)  
(anodes, for oxidn. of .beta.-cyanoethyl ethers)
- IT 1309-60-0  
RL: PRP (Properties)  
(anodes, for oxidn. of .beta.-cyanoethyl ethers)
- IT 7664-93-9, uses and miscellaneous  
RL: USES (Uses)  
(electrochem. oxidn. of .beta.-cyanoethyl ethers on lead dioxide or platinum in soln. contg.)
- IT 50-00-0P, preparation 74-90-8P, preparation 75-07-0P, preparation **109-78-4P** 6162-76-1P  
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in electrochem. oxidn. of .beta.-cyanoethyl ethers)
- IT 60-29-7, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidn. of, electrochem., on lead oxide or platinum)
- IT **110-67-8** **1656-48-0** **2141-62-0** 33573-94-3 **99764-73-5**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidn. of, electrochem., on lead oxide or platinum in sulfuric acid)
- IT 11129-89-8  
RL: PRP (Properties)

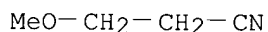
(platinum electrode contg., oxidn. of .beta.-cyanoethyl ethers on)  
IT 64-18-6P, preparation 64-19-7P, preparation **372-09-8P**  
RL: PREP (Preparation)  
(prepn. of, by electrochem. oxidn. of .beta.-cyanoethyl ethers)  
IT **7440-06-4**, uses and miscellaneous  
RL: USES (Uses)  
(anodes, for oxidn. of .beta.-cyanoethyl ethers)  
RN 7440-06-4 HCAPLUS  
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

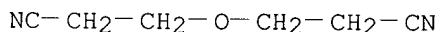
IT **109-78-4P**  
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in electrochem. oxidn. of .beta.-cyanoethyl ethers)  
RN 109-78-4 HCAPLUS  
CN Propanenitrile, 3-hydroxy- (9CI) (CA INDEX NAME)



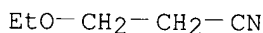
IT **110-67-8 1656-48-0 2141-62-0**  
**99764-73-5**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidn. of, electrochem., on lead oxide or platinum in sulfuric acid)  
RN 110-67-8 HCAPLUS  
CN Propanenitrile, 3-methoxy- (9CI) (CA INDEX NAME)



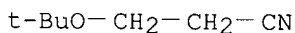
RN 1656-48-0 HCAPLUS  
CN Propanenitrile, 3,3'-oxybis- (9CI) (CA INDEX NAME)



RN 2141-62-0 HCAPLUS  
CN Propanenitrile, 3-ethoxy- (9CI) (CA INDEX NAME)



RN 99764-73-5 HCAPLUS  
CN Propanenitrile, 3-(1,1-dimethylethoxy)- (9CI) (CA INDEX NAME)



IT **372-09-8P**  
RL: PREP (Preparation)  
(prepn. of, by electrochem. oxidn. of .beta.-cyanoethyl ethers)  
RN 372-09-8 HCAPLUS  
CN Acetic acid, cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)

NC-CH<sub>2</sub>-CO<sub>2</sub>H

L42 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS  
AN 1985:614838 HCAPLUS  
DN 103:214838  
TI Anodic oxidation of 2-cyanoethanol to cyanoacetic acid  
AU Wermeckes, Bernd; Beck, Fritz  
CS GH, Univ. Duisburg, Duisburg, D-4100/1, Fed. Rep. Ger.  
SO Chemische Berichte (1985), 118(9), 3771-80  
CODEN: CHBEAM; ISSN: 0009-2940  
DT Journal  
LA German  
CC 23-16 (Aliphatic Compounds)  
Section cross-reference(s): 72  
OS CASREACT 103:214838  
AB 2-Cyanoethanol was oxidized electrochem. to cyanoacetic acid in aq. H<sub>2</sub>SO<sub>4</sub> at Pt and PbO<sub>2</sub> anodes (current densities of 30-200 mA cm<sup>-2</sup>). Current efficiencies and material yields were up to 60%. Side products were HCN (via an anodic attack at .beta.-CH<sub>2</sub>) and cyanoacetaldehyde, with 8-15 and 3-13% current efficiencies on Pt. In principle, HCN can be recycled to new starting material and cyanoacetaldehyde to yield further product. Electrooxidn. at Pt takes place at an anode which is partially covered with platinum oxides. High over-voltages are interpreted in terms of a voltage drop in a rigid org. adsorbate layer.  
ST hydroxypropanenitrile anodic oxidn electrochem  
IT Oxidation, electrochemical  
(of cyanoethanol to cyanoacetic acid)  
IT **109-78-4**  
RL: **RCT (Reactant); RACT (Reactant or reagent)**  
(anodic oxidn. of)  
IT 74-90-8P, preparation 6162-76-1P  
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in anodic oxidn. of cyanoethanol)  
IT **372-09-8P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, by anodic oxidn. of cyanoethanol)  
IT **109-78-4**  
RL: **RCT (Reactant); RACT (Reactant or reagent)**  
(anodic oxidn. of)  
RN 109-78-4 HCAPLUS  
CN Propanenitrile, 3-hydroxy- (9CI) (CA INDEX NAME)

HO-CH<sub>2</sub>-CH<sub>2</sub>-C≡N

IT **372-09-8P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, by anodic oxidn. of cyanoethanol)  
RN 372-09-8 HCAPLUS  
CN Acetic acid, cyano- (6CI, 8CI, 9CI) (CA INDEX NAME)

NC-CH<sub>2</sub>-CO<sub>2</sub>H